## **EAST Search History**

Ref #	Hits	Search Query	DBs	Default Operator	Plurals	Time Stamp
L1	786	(514/301,546/114).CCLS.	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT	OR	OFF	2007/12/12 11:12
L2	23	I1 and selectin	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT	OR	OFF	2007/12/12 11:12

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PASSWORD:

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         JUL 02
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         JUL 16 CAplus enhanced with French and German abstracts
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         JUL 18
                 CA/CAplus patent coverage enhanced
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         JUL 26
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        AUG 27
                 Full-text patent databases enhanced with predefined
                 patent family display formats from INPADOCDB
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                 1967-1998
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              AND CURRENT DISCOVER FILE IS DATED 19 SEPTEMBER 2007.
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FULL ESTIMATED COST

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chain nodes :

10 11 12 19 21 22 23 25 26 27 28

ring nodes :

1 2 3 4 5 6 7 8 9 13 14 15 16 17 18

ring/chain nodes :

20

chain bonds :

8-10 10-11 10-23 11-12 11-13 14-26 15-25 16-19 17-28 18-27 19-20 19-21

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9 13-14 13-18 14-15 15-16 16-17 17-18

exact/norm bonds :

1-2 1-6 2-3 3-4 4-5 5-6 8-10 10-11 11-12 16-19 19-20 19-21 19-22

exact bonds:

5-7 6-9 7-8 8-9 10-23 11-13 14-26 15-25 17-28 18-27

normalized bonds :

13-14 13-18 14-15 15-16 16-17 17-18

isolated ring systems :
containing 1 : 13 :

## Match level:

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS 11:CLASS 12:CLASS 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:CLASS 20:CLASS 21:CLASS 22:CLASS 23:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS

## L1 STRUCTURE UPLOADED

=> d 11

L1 HAS NO ANSWERS

L1 STR

Structure attributes must be viewed using STN Express query preparation.

=> s 11

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SAMPLE SCREEN SEARCH COMPLETED - 206 TO ITERATE

100.0% PROCESSED 206 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

50 ANSWERS

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PROJECTED ITERATIONS:

3259 TO 4981

PROJECTED ANSWERS:

3027 TO 4693

L2

50 SEA SSS SAM L1

=> s 11 full

FULL SEARCH INITIATED 11:15:04 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 3831 TO ITERATE

100.0% PROCESSED 3831 ITERATIONS

3524 ANSWERS

SEARCH TIME: 00.00.01

L3 3524 SEA SSS FUL L1

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ENTRY SESSION 172.10 172.31

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=> s 13 full

L4 3 L3

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L4 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:1331198 CAPLUS
DOCUMENT NUMBER: 146:184625
TITLE: 30 pharmacophore based virtus

146:184625
3D pharmacophore based virtual screening of T-type calcium channel blockers
Doddareddy, Munikumar Reddyr Choo, Hyunahr Cho, Yong
Seor Rhim, Hyewhon, Yoh, Hun Yeongr Lee, Jung-Har
Jeong, Seong-Woo, Pae, Ae Nim
Life Science Division, Korea Institute of Science and
Technology, Seoul, 130-650, S. Korea
Bioorganic & Medicinal Chemistry (2007), 15(2),
1091-1105 AUTHOR (S):

CORPORATE SOURCE:

SOURCE:

CODEN: BMECEP; ISSN: 0968-0896 Elsevier Ltd.

PUBLISHER: DOCUMENT TYPE: English LANGUAGE:

Virtual screening of the com. databases was done by using a three dimensional pharmacophore previously developed for T-type calcium channel blockers using CATALYST program. Biol evaluation of 25 selected virtual hits resulted in the discovery of a highly potent compound (1) with ICSO value of 0.10 µM, eight times as potent as the known selective T-type calcium channel blocker, mibefradil. Search for similar compds, yielded several hits with micro-molar ICSO values and high T-type calcium channel selectivity. Based on the structure of the virtual hits, small mol. libraries with novel scaffolds were designed, synthesis and biol. evaluation of which are currently in progress. This result shows a successful example of ligand based drug discovery of potent T-type calcium channel blockers.
449767-52-6
KL: PAC (Pharmacological activity), PRP (Properties), THU (Therapeutic use); BIOL (Biological study), USSS (Uses)
(30 pharmacophore based virtual screening of T-type calcium channel blockers)
449767-52-6 CAPIUS
Thieno[2,3-c]pyridine-3-carboxylic acid, 6-ethyl-4,5,6,7-tetrabydro-2-[[4-[(methylphenylamino)sulfonyl]benzoyl]amino]-, ethyl ester (CA INDEX NAME)

L4 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER:
DOCUMENT NUMBER: 2004:681500 CAPLUS
111.125321
111.125321
Pharmaceutical compositions comprising thieno[2,3-c]pyridines
Gregor, Pauls Harris, Nicholass Koppel, Jurajs Zhuk, Regina
Rimonym Pharmaceuticals Ltd., Israel
PCT Int. Appl., 87 pp.
CODEM: PIXKD2
Patent

Patent English 1

DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PAT	ent i	NO.			KIN		DATE				ICAT				D	ATE		
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PRIORITY											003-							
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OTHER SO	URCE	(5):			MAR	PAT	141:	1953:					•					

R SOURCE(S): MARPAT 141:195321
The present invention provides thieno(2,3-c]pyridines, and pharmaceutical compns. comprising thieno(2,3-c)pyridines. The compds. capable of inhibiting glycosaminoglycan (GAG) interactions with effector cell adhesion mods. (ECAM) are useful for treating diseases and disorders mediated by GAG-ECAMs interactions, particularly inflammatory and autoimmune diseases, viral diseases, cancer, and amyloid disorders. Thus, a capsule contained a thieno[2,3-c]pyridine 40.0, starch 109.0, and Mg stearate 1.0 mg.
533904-03-9P 738620-45-6P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); TRU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(Oses)
(pharmaceutical compns. comprising thieno[2,3-c]pyridines)
533904-03-9 CAFLUS
Thieno[2,3-c]pyridine-3-carboxamide, 6-ethyl-4,5,6,7-tetrahydro-N-methyl-2[[4-[(methylphenylamino)sulfonyl]benzoyl]amino]- (CA INDEX NAME)

ANSWER 1 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

REFERENCE COUNT:

26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 2 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

738620-45-6 CAPLUS Thieno[2,3-c]pyridine-3-carboxamide, 6-ethyl-4,5,6,7-tetrahydro-2-[[4-[(4-methyl-1-piperaxinyl)sulfonyl)benzoyl]amino]- (CA INDEX NAME)

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440334-81-6 449767-27-5 449767-88-e
449767-89-9 449768-16-5 449768-37-0
449768-51-8 449768-53-0 449768-37-0
449768-77-8 449768-83-6 449783-27-1
486455-13-8 486453-14-9 486453-16-1
486455-13-2 486453-22-9 486453-20-7
486453-25-2 486453-22-9 486453-24-1
486453-25-2 486453-26-9 486453-24-1
486453-25-6 489470-30-6 489470-38-4
488470-54-4 489470-89-5 489470-97-5
4884710-47-4 489471-11-6 489471-10-1
488471-10-7 489471-11-6 489471-16-1
489471-38-7 489471-39-6 889470-97-3
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- RN 449767-27-5 CAPLUS

  Thieno[2,3-c]pyridine-3-carboxamide, 4,5,6,7-tetrahydro-6-methyl-2-[{4-{(1,3,3-trimethyl-6-azabicyclo[3,2.1]oct-6-yl)sulfonyl]benzoyl]amino]-(CA INDEX NAME)
- Me NH-C-NF2 S-NMH-C-NF2
- RN 449767-88-8 CAPLUS
  CN Benzamide, N-[3-(2-benzothiazolyl)-6-ethyl-4,5,6,7-tetrahydrothieno[2,3-c]pyridin-2-yl]-4-[(diethylamino]sulfonyl]- (CA INDEX NAME)
- Et NH-C O
- RN 449767-89-9 CAPLUS
  CN Benzamide, N-[3-(2-benzothiazolyl)-6-ethyl-4,5,6,7-tetrahydrothieno[2,3-c]pyridin-2-yl]-4-[(butylethylamino)sulfonyl]- (CA INDEX NAME)
- L4 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
- i-Pr NH-C O Et | S-N-Bu-n | C-NH<sub>2</sub> | C-NH<sub>2</sub>
- RN 449768-53-0 CAPLUS
  CN Thieno[2,3-c]pyridine-3-carboxamide, 4,5,6,7-tetrahydro-6-{1-methylethyl}~
  2-[[4-[(methylphenylamino)sulfonyl]benzoyl]amino]- (CA INDEX NAME)
- 1-Pr NH-C Ph S-N-Me
- RN 449768-67-6 CAPLUS

  Thieno[2,3-c]pyridine-3-carboxamide, 2-[[4-[[3,5-dimethyl-1-piperidiny]]bulfony]benzoyl]amino]-4,5,6,7-tetrahydro-6-(1-methylethyl)-(CA INDEX NAME)
- 1-Pr NH-C NH2
- RN 449768-77-8 CAPLUS
  CN Thieno[2,3-c]pyridine-3-carboxamide, 2-[[4-[(3,4-dihydro-2(1H)-isoquinolinyl)sulfonyl]benzoyl]amino]-4,5,6,7-tetrahydro-6-(1-methylethyl)-(CA INDEX NAME)

L4 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

- RN 449768-16-5 CAPLUS
  CN Thieno(2,3-c)pyridine-3-carboxylic acid, 2-[{4[(butylmethylamino)sulfonyl)benzoyl)amino]-4,5,6,7-tetrahydro-6-(1methylethyl)-, ethyl ester (CA INDEX NAME)
- i-Pr NH-C OEt
- RN 449768-37-0 CAPLUS

  Thieno[2,3-c]pyridine-3-carboxylic acid, 2-[[4-[3,4-dihydro-1(2H)-quinclinyl]sulfonyl]benzoyl]amino]-4,5,6,7-tetrahydro-6-(1-methylethyl)-, ethyl ester (CA INDEX NAME)
- i-Pr NH- COEt
- RN 449768-51-8 CAPLUS
  CN Thieno[2,3-c]pyridine-3-carboxamide, 2-[[4-[(butylethylamino)sulfonyl]benz
  oyl]amino]-4,5.6,7-tetrahydro-6-(1-methylethyl)- (CA INDEX NAME)
- L4 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
- i-Pr NH-C S NH-C S NH-C S NH-C
- RN 449768-83-6 CAPLUS
  CN Benzamide, N-[3-(2-benzothiazolyl)-4,5,6,7-tetrahydro-6-(1-methylethyl)thieno[2,3-c]pyridin-2-yl]-4-[(diethylamino)sulfonyl]- (CAINOEX NAME)
- i-Pr S NH-C S-NEt2
- RN 449783-27-1 CAPLUS
  CN Thieno[2,3-c]pyridine-3-carboxylic acid, 2-[[4-[(hexahydro-1H-azepin-1-yl)sulfonyl)benzoyl]amino]-4,5,6,7-tetrahydro-5,5,7,7-tetramethyl-, ethylester (CA INDEX NAME)
- Me Me S NH-C OEt
- RN 486453-13-8 CAPLUS
  CN Benzamide, N-[3-(2-benzothiazolyl)-4,5,6,7-tetrahydro-6-methylthieno[2,3-c]pyridin-2-yl]-4-[(diethylamino)sulfonyl]- (CA INDEX NAME)

RN 486453-14-9 CAPLUS
CN Benzamide, N-[3-{2-benzothiazolyl}-4,5,6,7-tetrahydro-6-methylthieno[2,3-c]pyridin-2-yl]-4-{dipropylamino|sulfonyl}- (CA INDEX NAME)

RN 486453-16-1 CAPLUS
CN Benzamide, N-[3-(2-benzothiazoly1)-4,5,6,7-tetrahydro-6-methylthieno[2,3-c]pyridin-2-yl]-4-[(dibutylamino)sulfonyl]- (CA INDEX NAME)

RN 486453-17-2 CAPLUS
CN Benzamide, N-[3-{2-benzothiazolyl}-4,5,6,7-tetrahydro-6-methylthieno[2,3-c]pyridin-2-yl]-4-[(butylmethylamino)sulfonyl]- (CA INDEX NAME)

L4 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 486453-22-9 CAPLUS
CN Benzamide, N-[3-[2-benzothiazoly1)-4,5,6,7-tetrahydro-6-methylthieno[2,3-c]pyridin-2-yl]-4-[1-piperidinylsulfony1)- (CA INDEX NAME)

RN 486453-24-1 CAPLUS
CN Benzamide, N-[3-{2-benzothiazolyl}-4,5,6,7-tetrahydro-6-methylthieno[2,3-c]pyrdidn-2-yl]-4-{3-methyl-1-piperidinyl}sulfonyl]- (CA INDEX NAME)

RN 486453-25-2 CAPLUS
CN Benzamide, N-[3-(2-benzothiazolyl)-4,5,6,7-tetrahydro-6-methylthieno[2,3-c]pyridin-2-yl]-4-[(4-methyl-1-piperidinyl)sulfonyl]- (CA INDEX NAME)

RN 486453-18-3 CAPLUS
CN Benzamide, N-[3-(2-benzothiazolyl)-4,5,6,7-tetrahydro-6-methylthieno[2,3-c]pyridin-2-yl]-4-[(butylethylamino)sulfonyl]- (CA INDEX NAME)

RN 486453-20-7 CAPLUS
CN Benzamide, N-[3-(2-benzothiazolyl)-4,5,6,7-tetrahydro-6-methylthieno[2,3-c]pyridin-2-yl]-4-[(di-2-propenylamino)sulfonyl]- (9CI) (CA INDEX NAME)

RN 486453-21-8 CAPLUS
CN Benzamide, N-[3-(2-benzothiazoly1)-4,5,6,7-tetrahydro-6-methylthieno[2,3-c]pyridin-2-yl]-4-(1-pyrrolidinylsulfonyl)- (CA INDEX NAME)

L4 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 486453-26-3 CAPLUS
CN Benzamide, N-[3-{2-benzothiazoly1}-4.5,6,7-tetrahydro-6-methylthieno[2,3-c]pyridin-2-yl]-4-[(3,5-dimethyl-1-piperidinyl)sulfonyl]- (CA INDEX NAME)

RN 486453-27-4 CAPLUS
CN Benzamide, N-[3-(2-benzothiazoly1)-4,5,6,7-tetrahydro-6-methylthieno[2,3-c]pyridin-2-y1]-4-(4-morpholinylsulfony1)- (CA INDEX NAME)

RN 486453-29-6 CAPLUS
CN Benzamide, N-[3-(2-benzothiazolyl)-4,5,6,7-tetrahydro-6-methylthieno[2,3-c)pyridin-2-yl]-4-[[bis(2-methoxyethyl)amino]sulfonyl]- (CA INDEX NAME)

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- RN 489470-30-6 CAPLUS
  CN Benzamide, N-[3-(2-benzothiazoly1)-6-ethyl-4,5,6,7-tetrahydrothieno[2,3-c]pyridin-2-yl]-4-[(dipropylamino)sulfonyl]- (CA INDEX NAME)
- Et NH-C O
- RN 489470-38-4 CAPLUS
  CN Benzamide, N-{3-{2-benzothiazolyl}-6-ethyl-4,5,6,7-tetrahydrothieno[2,3-c]pyridin-2-yl]-4-{(di-2-propenylamino|sulfonyl]- (9CI) (CA INDEX NAME)
- Et NH- C OFFE CH2 CH2 CH2 CH2 CH2 CH2
- RN 489470-54-4 CAPLUS
  CN Benzamide, N-[3-(2-benzothiazoly1)-6-ethy1-4,5,6,7-tetrahydrothieno[2,3-c]pyridin-2-yl]-4-[(hexahydro-IH-azepin-1-yl)sulfony1)- (CA INDEX NAME)
- L4 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
- 1-Pr NH-C- S NH-C- CH2-CH2-CH2-CH2
- RN 489471-00-3 CAPLUS
  CN Benzamide, N-(3-(2-benzothiazoly1)-4,5,6,7-tetrahydro-6-(1-methylethyl)thieno[2,3-c]pyridin-2-yl]-4-(1-piperidinylsulfonyl)- (CA INDEX NAME)
- i-Pr NH-C NH-C NH-C
- RN 489471-01-4 CAPLUS

  Benzamide, N-[3-(2-benzothiazolyl)-4,5,6,7-tetrahydro-6-(1-methylathyl)thieno[2,3-c]pyridin-2-yl]-4-[(2-methyl-1-piperidinyl)sulfonyl]- (CA INDEX NAME)
- 1-Pr NH-C
- RN 489471-04-7 CAPLUS CN Benzamide, N-[3-(2-benzothiazoly1)-4,5,6,7-tetrahydro-6-(1-

L4 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

- RN 489470-89-5 CAPLUS

  Thieno[2,3-c]pyridine-3-carboxylic acid, 2-[[4-[[4-(ethoxycarbonyl)-1piperazinyl]sulfonyl]benzoyl]amino]-4,5,6,7-tetrahydro-6-(1-methylethyl)-,
  ethyl ester (CA INDEX NAME)
- i-Pr NH-C S NH-C C-OEt
- RN 489470-97-5 CAPLUS
  CN Benzamide, N-[3-(2-benzothiazolyl)-4,5,6,7-tetrahydro-6-(1-methylethyl)thieno[2,3-c]pyridin-2-yl]-4-[(butylethylamino)sulfonyl]- (CA INDEX NAME)
- i-Pr NH-C
- RN 489470-98-6 CAPLUS

  CN Benzamide, N-[3-(2-benzothiazolyl)-4,5,6,7-tetrahydro-6-[1-methylethyl) thieno[2,3-c]pyridin-2-yl]-4-[(di-2-propenylamino) sulfonyl]-(SCI) (CA INDEX NAME)
- L4 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN (Continued) methylethyl)thieno[2,3-c]pyridin-2-yl]-4-(4-morpholinylsulfonyl)- (CAINDEX NAME)
- i-Pr NH-C NH-C
- RN 489471-11-6 CAPLUS

  Thieno[2,3-c]pyridine-6(5H)-carboxylic acid, 3-(2-benzothiazolyl)-2-[[4[(diethylamino) sulfonyl]benzoyl]amino]-4,7-dihydro-, ethyl ester (CA
  INDEX NAME)
- BELO-C S NIH- C O O O
- RN 489471-16-1 CAPLUS

  Thieno[2,3-c]pyridine-3-carboxylic acid, 2-[[4-((di-2-propsy)lamino) sulfonyl]benzoyl]amino]-4,5,6,7-tetrahydro-5,5,7,7-tetramethyl-, methyl ester (9CI) (CA INDEX NAME)
- Me Me O CH2-CH=CH2

  HN S NH-C

  C-OMe
- RN 489471-25-2 CAPLUS
  CN Thieno[2,3-c]pyridine-3-carboxamide, 2-[[4-[(diethylamino)sulfonyl]benzoyl]amino]-4,5,6,7-tetrahydro-5,5,7,7-tetramethyl- (CA INDEX NAME).

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RN 489471-29-6 CAPLUS
CN Thieno[2,3-c]pyridine-3-carboxamide, 2-[[4-{[butylmethylamino]sulfonyi]ben zoyl]amino]-4,5,6,7-tetrahydro-5,5,7,7-tetramethyl- (CA INDEX NAME)

RN 489471-31-0 CAPLUS
CN Thieno[2,3-c]pyridine-3-carboxamide, 2-[[4-[(cyclohexylmethylamino)sulfony l]benzoyl]amino]-4,5,6,7-tetrahydro-5,5,7,7-tetramethyl- (CA INDEX NAME)

RN 489471-38-7 CAPLUS
CN 1-Piperazinecarboxylic acid, 4-[[4-[[3-(aminocarbonyl)-4,5,6,7-tetrahydro-5,5,7,7-tetrahethylthieno[2,3-c]pyridin-2-yl]amino]carbonyl]phenyl]sulfony l]-, ethyl ester (CA INDEX NAME)

L4 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 524706-73-8 CAPLUS

Benzamide, N-[3-(2-benzothiazolyl)-4,5,6,7-tetrahydro-6-methylthieno[2,3-c]pyridin-2-yl]-4-[(1,3,3-trimethyl-6-azabicyclo[3,2,1]oct-6-yl)sulfonyl]-(CA INDEX NAME)

RN 533895-61-3 CAPLUS

Thieno[2,3-c]pyridine-3-carboxamide, 2-[[4-[(3,4-dihydro-1(2H)-quinolinyl)sulfonyl]benzoyl]amino]-6-ethyl-4,5,6,7-tetrahydro-N-methyl-(CA INDEX NAME)

RN 533904-54-0 CAPLUS
CN Thieno[2,3-c]pyridine-3-carboxamide, 2-[[4-[(diethylamino)sulfonyl]benzoyl

Me Me S NH-C-OEt

RN 489471-39-8 CAPLUS

Thieno[2,3-c]pyridine-3-carboxamide, 2-[[4-[(3,4-dihydro-1(2H)-quinolinyl)sulfonyl]benzoyl}amino]-4,5,6,7-tetrahydro-5,5,7,7-tetramethyl-(CA INDEX NAME)

RN 524694-99-3 CAPLUS
CM Benzamide, N-[3-(2-benzothiazolyl)-4,5,6,7-tetrahydro-6(phenylmethyl)thieno[2,3-c]pyridin-2-yl]-4-[(diethylamino)sulfonyl]- (CA
INDEX NAME)

RN 524695-12-3 CAPLUS
CN Benzamide, N-[3-(2-benzothiazoly1)-4,5,6,7-tetrahydro-6-methylthieno[2,3-c]pyridin-2-yll-4-[[methylphenylamino]sulfonyl]- (CA INDEX NAME)

L4 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN (Continued) | amino]-6-ethyl-4,5,6,7-tetrahydro-N-methyl- (CA INDEX NAME)

RN 681264-20-0 CAPLUS
CN Benzanide, N-[3-(2-benzothiazolyl)-4,5,6,7-tetrahydro-5,5,7,7-tetramethyl.thieno[2,3-c]pyridin-2-yl]-4-(3,4-dihydro-1(2H)-quinolinyl)sulfonyl)- (CA INDEX NAME)

RN 681439-14-5 CAPLUS

Thieno[2,3-c]pyridine-3-carboxamide, 2-[[4-[(3,4-dihydro-2[H])-isoquinoliny]) sulfonyl]benzoyl]amino]-4,5,6,7-tetrahydro-5,5,7,7-tetramethyl- (CA INDEX NAME)

RN 681439-15-6 CAPLUS CN Thieno[2,3-c]pyridine-3-carboxamide, 2-[[4-[[bis(2ANSWER 2 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN (Continued) methoxyethyl) amino] sulfonyl]benzoyl]amino]-4,5,6,7-tetrahydro-5,5,7,7-tetramethyl- (CA INDEX NAME)

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738620-43-4 CAPLUS
1-Piperazinecarboxylic acid, 4-[[4-[[[3-(2-benzothiazoly1)-4,5,6,7-tetrahydro-6-methylthieno[2,3-c]pyridin-2-yl]amino]carbonyl]phenyl]sulfony
1]-, ethyl ester, monohydrochloride (9CI) (CA INDEX NAME)

● HC1

738620-44-5 CAPLUS
Thieno[2,3-c]pyridine-3-carboxamide, 6-ethyl-2-[[4[[ethyl:phenylmethyl]amino]sulfonyl]benzoyl]amino]-4,5,6,7-tetrahydro(CA INDEX NAME)

ANSWER 2 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

ANSWER 2 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN

738620-48-9 CAPLUS
Thieno[2,3-c]pyridine-3-carboxamide, 6-ethyl-4,5,6,7-tetrahydro-N-methyl-2[[4-[(4-methyl-1-piperazinyl) sulfonyl]benzoyl]amino] (CA INDEX NAME)

738620-49-0 CAPLUS Benzamide, N-(3-(2-benzothiazoly1)-6-ethy1-4,5,6,7-tetrahydrothieno[2,3-c]pyridin-2-y1]-4-[(4-methyl-1-piperaziny1)sulfony1]-, monohydrochloride (SCI) (CA INDEX NAME)

• HC1

738620-50-3 CAPLUS
Thieno[2,3-c]pyridine-3-carboxamide, 2-[[4-[(diethylamino)sulfonyl]benzoyl
]amino]-6-ethyl-4,5,6,7-tetrahydro-N-4-morpholinyl- (CA INDEX NAME)

L4 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:826913 CAPLUS
COCUMENT NUMBER: 139:49321
TITLE: Property-based design of GPCR-targeted library
Balakin, Konstantin V.; Tkachenko, Sergey E.; Lang,
Stanley A.; Okun, Ilya; Ivashchenko, Andrey A.;
Savchuk, Nikolay P.
CORPORATE SOURCE: Chemical Diversity Labs Inc., San Diego, CA, 92121,
USA
SOURCE: Journal of Chemical Information and Computer Sciences
(2002), 42(6), 1332-1342
CODEN; JCISDB; ISSN: 0055-2338
PUBLISHER: American Chemical Society
Journal
LANGUAGE: English
AB The design of a GPCR-targeted library, based on a scoring scheme for the
classification of mois. into "GPCR-ligand-like", is outlined. The methodol. is a valuable tool that can aid in the
selection and prioritization of potential GPCR ligands for bioscreening
from large collections of compds. It is based on the distillation of
knowledge
from large databases of GPCR and non-GPCR active agents. The method
employed a set of descriptors for encoding the mol. structures and by
training of a neural network for classifying the mols. The mol.
requirements were profiled and validated by using available databases of
GPCR- and non-GPCR-active agents. The method enables efficient
qualification or disqualification of a mol. as a potential GPCR ligand and
represents a useful tool for constraining the size of GPCR-active
drugs.

IT 478932-86-4

libraries that will help speed up the development of new GPCR-active drugs.
478932-86-4
KL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(property-based design of GPCR-targeted library)
478932-86-4 CAPLUS
Thieno[2,3-c]pyridine-3-carboxylic acid, 6-ethyl-4,5,6,7-tetrahydro-2-[[4-[(4,6,6-trimethyl-2-azabicyclo[2.2.1]hept-2-yl)sulfonyl]benzoyl]amino]-, ethyl ester (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT 22

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(FILE 'HOME' ENTERED AT 11:14:33 ON 12 DEC 2007)

FILE 'REGISTRY' ENTERED AT 11:14:43 ON 12 DEC 2007

L1 STRUCTURE UPLOADED

L2 50 S L1

L3 3524 S L1 FULL

FILE 'CAPLUS' ENTERED AT 11:15:11 ON 12 DEC 2007

L4 3 S L3 FULL

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